Notes on spectral clusters for semiclassical Schrodinger operators (Spectral and Scattering Theory and Related Topics)

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Notes on spectral clusters for semiclassical Schrödinger operators

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Abstract

In this short note, we discuss the relationships between eigenvalues of Schrödinger operators and periodic trajectories of classical mechanics. For a Hamiltonian function $H(x,p) : T^*\mathbf{R}^n \to \mathbf{R} \cup \{\pm\infty\}$, let $\widehat{H} \equiv Op_h^W(H(x,p))$ be a self-adjoint Weyl type pseudo-differential operator and $\mathrm{Spec}(\widehat{H})$ be the spectrum of $\widehat{H}$. If $\Lambda_h(E,c) = \mathrm{Spec}(\widehat{H}) \cap [E-c, E+c]$ consists of only eigenvalues, we define the (semiclassical) essential difference spectrum by

$$D\sigma(\hat{H}) \equiv \overline{\{\frac{E_i(h)-E_j(h)}{h} \mid E_i(h), E_j(h) \in \Lambda_h(E,c)\}}^{\mathrm{ess}} \subset \mathbf{R}$$

where $\overline{\{\cdot\}}^{\mathrm{ess}}$ means the set of accumulating points as $h \to 0$. We prove the so-called Helton type theorem including Hamiltonians with singular potentials, that is, either every classical Hamiltonian flow is periodic near E or $D\sigma(\hat{H}) = \mathbf{R}$.

1 Introduction

Let us first recall the Helton theorem. For a compact oriented, smooth Riemannian n-dimensional manifold (M,g), we set the classical mechanics and quantum mechanics by

$$(\mathrm{QP}) \begin{cases} -\triangle u_j(x) = \lambda_j u_j(x), \\ \{u_j(x),\ \lambda_j\} : \text{Eigenfunction expansion}, \end{cases}$$

$$(\mathrm{CP}) \begin{cases} X_H = (\frac{\partial H}{\partial p}, -\frac{\partial H}{\partial x}), \\ \exp tX_H : S^*M \to S^*M : \text{Geodesic flow}, \end{cases}$$

where $\triangle$ denotes the Laplacian and $H(x,p) = \sqrt{g_{st}(p,p)} \in C^\infty(T^*M)$. We note that $\triangle = \frac{1}{\sqrt{g}}\frac{\partial}{\partial x_i}\{\sqrt{g}g^{ij}\frac{\partial}{\partial x_j}\}$ and $H(x,p) = \sqrt{g_{st}(p,p)} = \sqrt{g^{ij}p_ip_j} \in C^\infty(T^*\mathbf{R}^n)$ on local charts. Under these circumstances, Helton proved [8] that either $D\sigma(\sqrt{-\triangle}) = \mathbf{R}$ or every geodesic curve of (CP) is closed. Here

$$D\sigma(\sqrt{-\triangle}) \equiv \overline{\{\sqrt{\lambda_i} - \sqrt{\lambda_j} \mid \lambda_i, \lambda_j \in \mathrm{Spec}(-\triangle)\}}^{\mathrm{ess}}$$

and $\overline{\{\cdot\}}^{\mathrm{ess}}$ means the set of accumulating points in $\mathbf{R}$. To understand the meaning of this theorem, we shall see three examples :
(Example 1) Let $(S^2,\ g_{st})$ be a standard 2-dim sphere in $\mathbf{R}^3$. Then $\lambda_j = j(j+1)$ with multiplicity $2j+1$ and

$$D\sigma(\sqrt{-\triangle}) = \mathbf{Z}.$$

(Example 2) Let $(M,\ g)$ be a 2-dim Zoll surface with period 2π. It is known (See e.g. [9, Lemma 29.2.1]) that $\sqrt{\lambda_j} = j + \frac{1}{2} + O(j^{-1})$ $j \in \mathbf{N}$ and

$$D\sigma(\sqrt{-\triangle}) = \mathbf{Z}.$$

(Example 3) Let $(\mathbf{R}^2/(2\pi\mathbf{Z})^2,\ g_{flat})$ be a 2-dim flat torus. Then $\lambda_{j,k} = j^2 + k^2$ $j,k \in \mathbf{N}$ and so

$$D\sigma(\sqrt{-\triangle}) = \mathbf{R}.$$

Every geodesic flow is periodic in Example 1 and 2, however, we find some geodesic curves are not closed in Example 3. These faithfully reflect properties of the difference specturm $D\sigma(\sqrt{-\Delta})$. We also would like to mention some recent results for compact manifold cases. For the case of magnetic Schrödinger operators (which is called Bochner Laplacian), the analogous result is given by R. Kuwabara [11], and if the periodic points of Hamiltonian with a smooth scalar potential have measure 0 on the energy surface $H^{-1}(e)$, T. Tate [15] proved $D_e\sigma(\sqrt{-\Delta}) = \mathbf{R}$.

It is emphasized that manifolds are compact and the potentials are not singular in the above theorems. So our purpose is to consider Hamiltonians including singular potentials on Euclidean spaces. Such a situation allows us to treat Hydrogen atoms and celestial mechanics. To do this, we set (SP) and (CP) by

$$
(\mathrm{SP})\begin{cases}\widehat{H}u_j(x,h) = E_j(h)u_j(x,h),\\ \{u_j(x,h),\ E_j(h)\} : \text{Eigenfunctions and eigenvalues,}\end{cases}
$$

$$
(\mathrm{CP})\begin{cases}X_H = (\frac{\partial H}{\partial p}, -\frac{\partial H}{\partial x}),\\ \exp tX_H : T^*\mathbf{R}^n \to T^*\mathbf{R}^n : \text{Hamiltonian flow,}\end{cases}
$$

where $H(x,p) : T^*\mathbf{R}^n \to \mathbf{R} \cup \{\pm\infty\}$ denotes a Hamiltonian function. Under suitable conditions (See §2), $\Lambda_h(E,c) = \mathrm{Spec}(\widehat{H}) \cap [E-c, E+c]$ consists of only eigenvalues and $\sharp\Lambda_h(E,c) \to \infty$ as $h \to 0$. Thus the semi-classical difference spectrum can be defined by

$$
D\sigma(\hat{H}) \equiv \overline{\{\frac{E_i(h)-E_j(h)}{h} \mid \lambda_i(h), \lambda_j(h) \in \Lambda_h(E,c)\}}^{\mathrm{ess}} \subset \mathbf{R}.
$$

Our result is analogous to the Helton theorem, that is, either every complete Hamiltonian flow is periodic near E or $D\sigma(\hat{H}) = \mathbf{R}$ (Theorem 2.5). Here the terminology "near E" will be explained in Sect. 3.

2 Semiclassical operators on $\mathbb{R}^n$

Let $A(x,p) \in L^1_{loc}(T^*\mathbb{R}^n)$ be a symbol. We define the Weyl type pseudo-differential operators by :

Definition 2.1.

$$
\hat{A}f(x) \equiv Op_h^W(A)f(x) \equiv \frac{1}{(2\pi h)^n}\int_{T^*\mathbb{R}^n} e^{\frac{i(x-y)\cdot p}{h}} A\left(\frac{x+y}{2}, p\right) f(y)\, dydp \quad \text{for } f(x) \in C_0^\infty(\mathbb{R}^n).
$$

Followings are the typical examples of Weyl type peudodifferential operators :

(Example 4)

$$
H(x,p) = xp \in C^\infty(T^*\mathbf{R}^n) \Rightarrow Op_h^W(H) = \frac{h}{2i}(x\partial_x + \partial_x x).
$$

(Example 5)

$$
H(x,p) = |p - A(x)|^2 + V(x) \Rightarrow Op_h^W(H) = |\frac{h}{i}\nabla - A(x)|^2 + V(x).
$$

(Example 6)

$$
H(x,p) = \frac{1}{2}|p|^2 - \frac{1}{|x|} \in L^1_{loc}(T^*\mathbf{R}^3) \Rightarrow Op_h^W(H) = -\frac{h^2}{2}\Delta - \frac{1}{|x|}.
$$

We assume that

(A1) $\hat{H}_h = Op_h^W(H)$ is essentially self-adjoint in $L^2(\mathbf{R}^n)$ for small $h > 0$.

(A2) $\Lambda_h(E,c) \equiv \mathrm{Spec}(\hat{H}_h) \cap [E-c, E+c]$ consists of asymptotically infinite many eigenvalues for small $h > 0$.

Our guiding principle is based on harmonic oscillators, hydrogen atoms and magnetic Schrödinger operators. In these cases, (A1) and (A2) are satisfied (See for instance [4, §4] and [13]).

Definition 2.2 (Semiclassical essential difference spectrum near E)**.** Under the assumptions (A1) and (A2),

$$
D\sigma(\hat{H}) \equiv \overline{\{\frac{E_i(h)-E_j(h)}{h} \mid E_i(h), E_j(h) \in \Lambda_h(E,c)\}}^{\mathrm{ess}}
$$

where $\overline{\{\cdot\}}^{\mathrm{ess}}$ means the set of accumulating points as $h \to 0$ (i.e. $a \in D\sigma(\hat{H})$ means that $\exists\frac{E_i(h)-E_j(h)}{h} \to a$ as $h \to 0$).

In this note we further assume that

(A3) $H(x,p)=\sum_{|\alpha|\le m} a_\alpha(x)p^\alpha$: real valued.

(A4) $\partial_x^\beta a_\alpha(x)\in L^1_{loc}(\mathbb{R}^n)\quad \forall\,|\beta|\le|\alpha|$.

(A5) $\exists$ finite set $K\in\mathbb{R}^n$ and $\rho>0$ such that a_α is analytic in

$$G_K\equiv\{|\mathrm{Im}\,x|<\rho,\ \mathrm{Re}\,x\notin K\}$$

and for some $C>0$ and $M>0$,

$$|a_\alpha(x)|\leqq C(1+|x|)^M\quad \text{in } G_K.$$

(A6) $\exp tX_H: H^{-1}(E-c,E+c)\to H^{-1}(E-c,E+c)$ is almost complete.

(i.e. $\exists\, S\subset H^{-1}(E-c+E+c)$ such that the Liouville measure of S^c is 0 and $\exp tX_H$ is complete on S).

We use the notion of Gevrey class : Given $\Omega\subset T^*\mathbb{R}^n$ and $s\geqq 1$, the Gevrey class G^s (of index s) is defined as the set of all functions $f\in C^\infty(\Omega)$ such that for every compact subset K there exists a $C=C_{f,K}$ satisfying

$$\max_{x\in K}|\partial^\alpha f(x)|\leqq C^{|\alpha|+1}(|\alpha!|)^s,\quad \forall\alpha\in\mathbb{Z}^n_+, |\alpha|=\alpha_1+\ldots+\alpha_n.$$

For $s>1$, $G^s_0(\Omega)=G^s(\Omega)\cap C_0^\infty(\Omega)$ contains non-zero functions. It is also known [1] that nice partitions of unity are constructed in suitable $s>1$. Under the assumptions (A1)$\sim$(A6), we have Egorov type theorem for Gevrey class symbols (See e.g. [2]).

Lemma 2.3. Let Ω be a bounded open subset of $T^*\mathbf{R}^n$ such that $\overline{\Omega}$ is $\exp tX_H$ invariant for every $t\in\mathbf{R}$ and $\overline{\Omega}\backslash(K\times\mathbf{R}^n)$. If supp$A\subset\Omega$ and A is Gevrey $s>1$, then

$$e^{-\frac{it\hat{H}}{h}}Op_h^W(A)e^{\frac{it\hat{H}}{h}}=Op_h^W((\exp tX_H)^*A)\quad \mod h.$$

By integrating with respect to t, we obtain

Corollary 2.4. Under the same assumptions of Lemma 2.3, if $\tilde{f}(t)\in C_0^\infty(\mathbb{R})$ then

$$A_f^R\equiv\int_{-R}^R\tilde{f}(t)e^{-\frac{it\hat{H}}{h}}Op_h^W(A)e^{\frac{it\hat{H}}{h}}dt=Op_h^W\left(\int_{-R}^R\tilde{f}(t)(\exp tX_H)^*Adt\right)\quad \mod h.$$

where $\tilde{f}(t)$ denotes the Fourier transform of $f(t)$ and $(\exp tX_H)^*A(x,p)=A(\exp tX_H(x,p))$ is the pull-back of A.

The analogy of Helton theorem for the smooth Hamiltonians is proved by M. Combescure and D. Robert [3]. Our purpose is to treat singular potentials :

Theorem 2.5. Under the assumptions (A1)$\sim$(A6), Either $D\sigma(\hat{H})=\mathbf{R}$ or every complete Hamiltonian flow on $H^{-1}((E-c,E+c))$ is periodic.

3 Outline of the proof of Theorem 2.5

Proof. Let $\tilde{f}\in C_0^\infty(\mathbb{R}_t)$ be a Fourier transform of $f(x)$. Assuming (A2), we have unitary operators $e^{\frac{it\hat{H}}{h}}$ by Stone's theorem [16]. We denote the spectral decomposition by $e^{\frac{it\hat{H}}{h}}=\sum_j e^{\frac{i}{h}E_j(h)t}P_j$ near E. Thus for a suitable Gevrey class symbol A with supp$A\subset H^{-1}(E-c,E+c)$,

$$\widehat{A}_f\equiv\int_{\mathbb{R}_t}\tilde{f}(t)e^{-\frac{it\hat{H}}{h}}Op_h^W(A)e^{\frac{it\hat{H}}{h}}dt \tag{1}$$

$$=\sum_{i,j}\int_{\mathbb{R}_t}\tilde{f}(t)e^{\frac{i}{h}(E_j(h)-E_i(h))t}P_iOp_h^W(A)P_jdt. \tag{2}$$

If $\sigma \notin D\sigma(\hat{H})$, there exists a sub interval $I_\sigma \in \Lambda_h(E,c)$ such that I_σ contains finite number $\frac{E_j(h)-E_i(h)}{h}$'s for small h. So if supp$\tilde{f} \subset I_\sigma$, $\widehat{A}_f$ is a finite rank h^∞ smoothing operator. By Corollary 2.4, we have

$$A_f^R \equiv \int_{-R}^{R} \tilde{f}(t)e^{-\frac{it\hat{H}}{h}} Op_h^W(A)e^{\frac{it\hat{H}}{h}}dt \tag{3}$$

$$= Op_h^W\left(\int_{-R}^{R} \tilde{f}(t)(\exp tX_H)^* A dt\right) \quad \mod h. \tag{4}$$

We note that

$$A_f^R - A_f = 0 \quad (\mathrm{mod}\ h) \text{ for large } R. \tag{5}$$

Considering the classical mechanics (CP), (A6) assures $X = \frac{1}{i}X_H$ is essentially self-adjoint in $L^2(S)$. Here $S \subset H^{-1}(E-c, E+c)$ denotes the subset on which $\exp tX_H$ is complete. From (4) and (5), the leading symbol of A_f satisfies

$$\begin{aligned}\int_{\mathbb{R}_t} \tilde{f}(t)(\exp tX_H)^* A dt &= \int_{\mathbb{R}_t} \tilde{f}(t)(e^{it(\frac{1}{i}X_H)})A dt \\ &= f(X)A(x,p) = 0 \\ &\quad \text{for all } A(x,p) \text{ (with supp}(A) \subset H^{-1}(E-c,E+c)\backslash(K\times\mathbb{R}^n)).\end{aligned}$$

Thus $f(X) = 0$, that is, $I_\sigma \cap \mathrm{Spec}(S) = \emptyset$ and so $\mathrm{Spec}(S) \subset D\sigma(\hat{H})$. We need the following lemma :

Lemma 3.1. (Spectrum of X) Either $\mathrm{Spec}(X) = \mathbb{R}$ or every Hamiltonian flow on S is periodic.

For the proofs of this lemma, see e.g. [7]. Thus $D\sigma(\hat{H}) \neq \mathbb{R}$ means that $\mathrm{Spec}(X) \neq \mathbb{R}$ and every Hamiltonian flow on S is periodic. □

4 Examples

In this section we introduce concrete examples. These examples are fundamental physical objects of quantum mechanics (See e.g. [14]).
(Example 7) (2-dim Harmonic oscillator)
Let $H(x,p) = \frac{1}{2}|p|^2 + Ax_1^2 + Bx_2^2$ $(A, B > 0)$. Then $\mathrm{Spec}(\hat{H}_h) = \{\sqrt{2A}(i+\frac{1}{2})h + \sqrt{2B}(j+\frac{1}{2})h \mid i,j \in \mathbf{N}_{\geqq 0}\}$.
For fixed $c > 0$ (even in the case $c = h^{1-\delta}$),

$$\begin{cases} D\sigma(\hat{H}) \neq \mathbf{R} & \text{for } \sqrt{\frac{B}{A}} \in \mathbf{Q}, \\ D\sigma(\hat{H}) = \mathbf{R} & \text{for } \sqrt{\frac{B}{A}} \notin \mathbf{Q}. \end{cases}$$

We compare $D\sigma(\hat{H})$ with the classical mechanics : For $\Sigma_E = \{(x,p) \in T^*(\mathbf{R}^n) |\ H(x,p) = E\}$, the Hamiltonian flow $\exp tX_H : \Sigma_E \to \Sigma_E$ satisfies

$$\begin{cases} \exp tX_H \text{ is always periodic for } \sqrt{\frac{B}{A}} \in \mathbf{Q}, \\ \exp tX_H \text{ is non-periodic} \quad \text{for } \sqrt{\frac{B}{A}} \notin \mathbf{Q}. \end{cases}$$

(Example 8)(Hydrogen atom) Let $H(x,p) = \frac{1}{2}|p|^2 - \frac{1}{r}$. Then $\mathrm{Spec}(\hat{H}_h) \cap \mathbf{R}_- = \{E_j(h) = -\frac{1}{2h^2j^2} \mid n \in \mathbf{N}_{>0}\}$.
For instance, taking $\Lambda(-1.5, 0.5)$ (i.e. $-2 < E_j(h) < -1$), we have

$$-2 < E_j(h) < -1 \Leftrightarrow -2 < -\frac{1}{2h^2j^2} < -1 \Leftrightarrow \frac{1}{2h} < j < \frac{1}{\sqrt{2h}}.$$

$$\begin{aligned}\left|\frac{E_{j_1}(h) - E_{j_2}(h)}{h}\right| &= \frac{1}{2h^3}\left|\frac{1}{j_1^2} - \frac{1}{j_2^2}\right| \\ &\geqq \frac{1}{2h^3}\left|\frac{1}{j_1^2} - \frac{1}{(j_1+1)^2}\right| \\ &> \frac{1}{2h^3}\left|\frac{1}{(\frac{1}{\sqrt{2h}})^2} - \frac{1}{(\frac{1}{\sqrt{2h}}+1)^2}\right| \\ &> \frac{2h+2\sqrt{2}}{2h^2+2\sqrt{2}h+1} \to 2\sqrt{2} \quad \text{as } h \to 0.\end{aligned}$$

It follows $D\sigma(\hat{H}) \neq \mathbf{R}$.

Regarding the classical mechanics whose orbits are all closed, followings are typical theorems.

Theorem 4.1 (J. Bertrand (1873)). Define 3-dim Hamiltonian with central force by $H(x,p) = \frac{1}{2}|p|^2 + V(r)$. If all bound orbits are also closed orbits, then $V(r) = \frac{A}{r}$ or $V(r) = Br^2$.

Theorem 4.2 ([12]). Let $H(x_1, x_2, p_1, p_2) = \frac{1}{2}|p|^2 + U(x_1) + U(x_2)$ where $U(x) = (\alpha^2 - \beta^2)^{-2}\{\alpha x - \beta[x^2 + \gamma(\alpha^2 - \beta^2)^{1/2}]\}^2$. For suitable α, β, γ, every Hamiltonian flow for low energy is all periodic.

One can apply Theorem 2.5 for quantum mechanics with above potentials. Many other systems are known, such as three charged particles with magnetic field [10], Lotka-Volterra system [6] $H(x,p) = \sum_{i=1}^{n}(r_i x_i - \exp(p_i + \frac{1}{2}\sum_{j=1}^{n} a_{ij}x_j))$ and etc.

5 Remark

The assumption (A5) is too strong. We can replace (A5) by

(A5)′ $\exists$ finite set $K \in \mathbb{R}^n$, a bounded subset $L \supset K$ and $\rho > 0$ s.t. $a_\alpha \in C^\infty(T^*\mathbb{R}^n)$ is analytic in

$$G_{L\backslash K} \equiv \{|\mathrm{Im}\, x| < \rho,\ \mathrm{Re}\, x \in L\backslash K\}$$

and for some $C > 0$ and $M > 0$,

$$|a_\alpha(x)| \leqq C(1+|x|)^M \quad \text{in } G_{L\backslash K}.$$

Let us introduce two C^∞-cutoff functions χ and ζ, where ζ is supported in a small neighborhood of $T^*\mathbb{R}^n\backslash(K \times \mathbb{R}^n)$ and $\chi = 1$ on supp ζ. The distance between the supports of ζ and $1-\chi$ is then positive. Consider the pseudodifferential operator $\widehat{A}$ with symbol $\mathrm{supp}A \subset \mathrm{T^*\mathbb{R}^n\backslash(K \times \mathbb{R}^n)}$ and write the commutator $[\widehat{H}, \widehat{A}]$ as follows :

$$[\widehat{H}, \widehat{A}] = [\widehat{H}, \widehat{A}]\chi + \widehat{H}\zeta\widehat{A}(1-\chi) + [\widehat{H}(1-\zeta), \widehat{A}](1-\chi).$$

In the last term of the right-hand side, each operator has a smooth symbol so that we can use the same computations as in the C^∞ pseudodiferential operators. The first terms give negligible contributions. Since

$$\|[\widehat{H}, \widehat{A}]\chi\|_{L^2} + \|\widehat{H}\widehat{A}(1-\chi)\|_{L^2} \leqq Ch.$$

The standard proof techniques of Egorov theorem are applicable (See [2] for more precise). Thus taking suitable partitions of unitiy of A, we obtain the Egorov theorem as in Lemma 2.3.

6 Conclusion

Simple Helton like theorems are discussed including when singular potentials. It is emphasized that the periods of closed orbits will be explicitly characterized by $D\sigma(\widehat{H})$ for the smooth potentials (See e.g. [5]). By using Kustaanheimo-Stiefel transforms, the Hamiltonians with coulombic potentials are presumed to have the same properties. We would like to mention about it in the future.

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